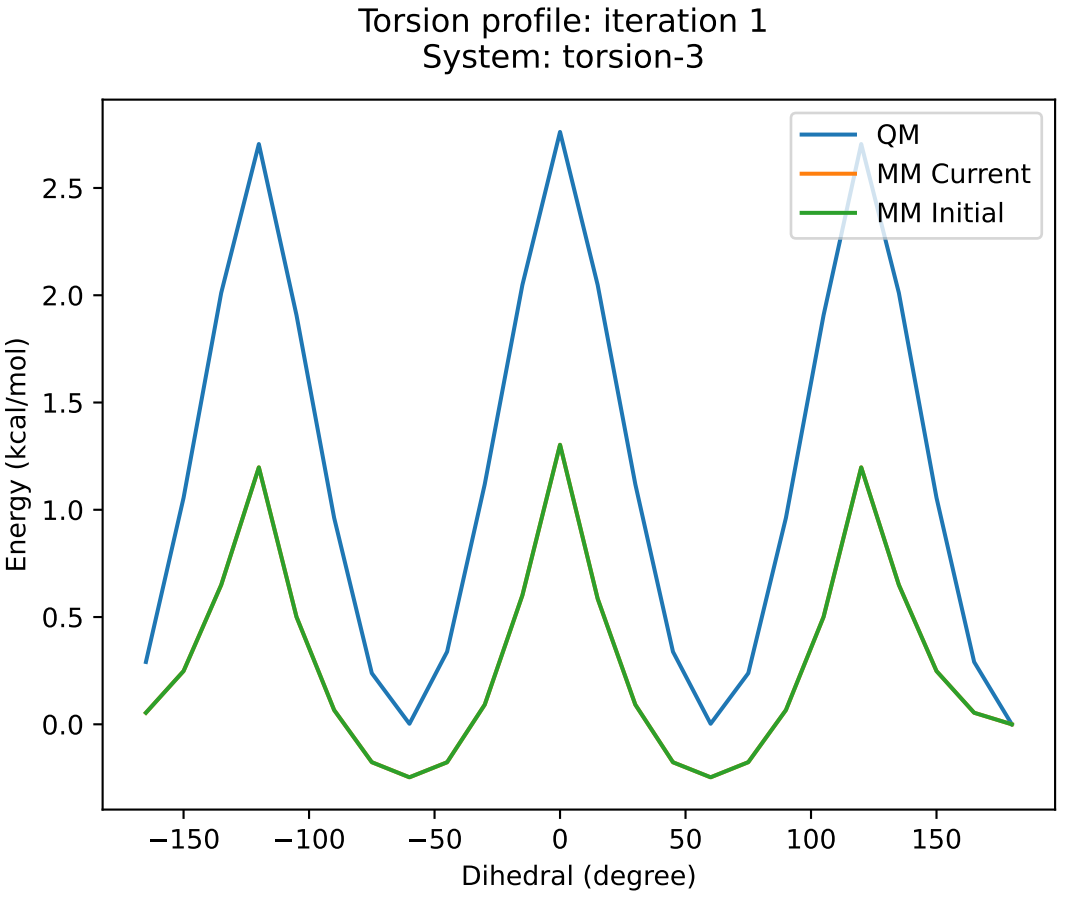
Torsion profile: iteration 1
System: torsion-3
QM
MM Current
MM Initial
Energy (kcal/mol)
2.5
2.0
1.5
1.0
0.5
0.0
−150
−100
−50
0
50
100
150
Dihedral (degree)